



# wwPDB X-ray Structure Validation Summary Report

Sep 21, 2014 – 05:20 AM EDT

PDB ID : 4OQ9  
Title : Satellite Tobacco Mosaic Virus Refined to 1.4 Å Resolution using non-crystallographic symmetry restraints  
Authors : Larson, S.B.; Day, J.S.; McPherson, A.  
Deposited on : 2014-02-07  
Resolution : 1.45 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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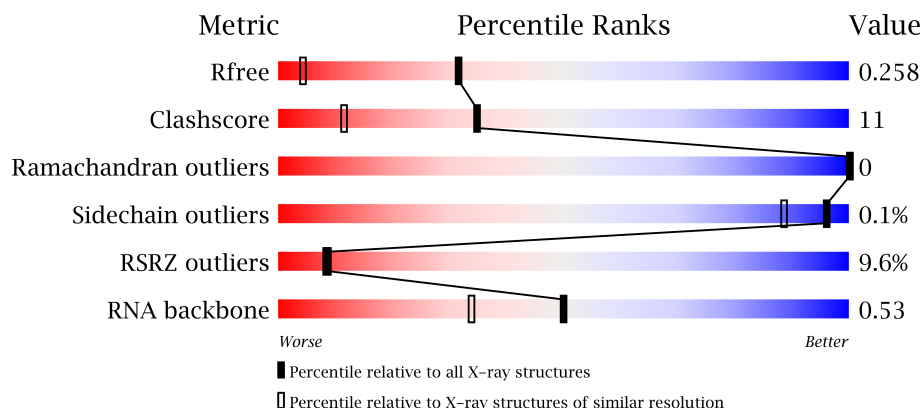
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23489
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 1.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2476 (1.50-1.42)
Clashscore	79885	2834 (1.50-1.42)
Ramachandran outliers	78287	2769 (1.50-1.42)
Sidechain outliers	78261	2767 (1.50-1.42)
RSRZ outliers	66119	2477 (1.50-1.42)
RNA backbone	1838	1002 (2.92-0.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	159	
1	B	159	
1	C	159	
1	D	159	
1	E	159	
1	F	159	
1	G	159	
1	H	159	
1	I	159	
1	J	159	
1	K	159	








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Mol	Chain	Length	Quality of chain
1	L	159	
1	M	159	
1	N	159	
1	O	159	
2	P	10	
2	Q	10	
2	R	10	
2	S	10	
2	T	10	
2	U	10	
2	V	10	
2	W	10	
2	X	10	
2	Y	10	
2	Z	10	
2	a	10	
2	b	10	
2	c	10	
2	d	10	
3	e	10	
3	f	10	
3	g	10	
3	h	10	
3	i	10	
3	j	10	
3	k	10	
3	l	10	
3	m	10	
3	n	10	
3	o	10	
3	p	10	
3	q	10	
3	r	10	
3	s	10	
4	1	2	
4	2	2	
4	3	2	
4	4	2	
4	5	2	
4	6	2	
4	7	2	
4	8	2	

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Mol	Chain	Length	Quality of chain
4	t	2	
4	u	2	
4	v	2	
4	w	2	
4	x	2	
4	y	2	
4	z	2	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	PO4	A	201[A]	-	X
5	PO4	A	201[B]	-	X
5	PO4	A	201[C]	-	X
5	PO4	A	201[D]	-	X
5	PO4	A	201[E]	-	X
5	PO4	H	201[A]	-	X
5	PO4	H	201[B]	-	X
5	PO4	H	201[C]	-	X
5	PO4	H	201[D]	-	X
5	PO4	H	201[E]	-	X
5	PO4	N	201[A]	-	X
5	PO4	N	201[B]	-	X
5	PO4	N	201[C]	-	X
5	PO4	N	201[D]	-	X
5	PO4	N	201[E]	-	X
6	SO4	A	202	-	X
6	SO4	B	201	-	X
6	SO4	C	201	-	X
6	SO4	D	201	-	X
6	SO4	E	201[A]	-	X
6	SO4	E	201[B]	-	X
6	SO4	E	201[C]	-	X
6	SO4	E	201[D]	-	X
6	SO4	E	201[E]	-	X
6	SO4	F	201	-	X
6	SO4	G	201[A]	-	X
6	SO4	G	201[B]	-	X
6	SO4	G	201[C]	-	X
6	SO4	G	201[D]	-	X
6	SO4	G	201[E]	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	SO4	G	202	-	X
6	SO4	H	202	-	X
6	SO4	I	201	-	X
6	SO4	J	201	-	X
6	SO4	K	201	-	X
6	SO4	L	201	-	X
6	SO4	M	201[A]	-	X
6	SO4	M	201[B]	-	X
6	SO4	M	201[C]	-	X
6	SO4	M	201[D]	-	X
6	SO4	M	201[E]	-	X
6	SO4	M	202	-	X
6	SO4	N	202	-	X
6	SO4	O	201	-	X
7	NA	A	203[A]	-	X
7	NA	B	203	-	X
7	NA	C	202[B]	-	X
7	NA	D	202	-	X
7	NA	E	204	-	X
7	NA	E	205	-	X
7	NA	F	203	-	X
7	NA	G	203	-	X
7	NA	H	203	-	X
7	NA	I	202[A]	-	X
7	NA	J	202[A]	-	X
7	NA	K	203[B]	-	X
7	NA	L	202	-	X
7	NA	M	203[B]	-	X
7	NA	N	203[A]	-	X
7	NA	O	202[B]	-	X
8	MG	E	203	-	X
8	MG	K	202	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 29296 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	15	0
			1201	761	213	219	8			
1	B	144	Total	C	N	O	S	0	14	0
			1191	753	210	219	9			
1	C	144	Total	C	N	O	S	0	18	0
			1204	768	210	217	9			
1	D	144	Total	C	N	O	S	0	19	0
			1223	779	215	220	9			
1	E	144	Total	C	N	O	S	0	16	0
			1211	768	214	220	9			
1	F	144	Total	C	N	O	S	0	18	0
			1216	775	214	218	9			
1	G	144	Total	C	N	O	S	0	16	0
			1198	760	210	219	9			
1	H	144	Total	C	N	O	S	0	17	0
			1205	766	210	221	8			
1	I	144	Total	C	N	O	S	0	16	0
			1201	762	210	220	9			
1	J	144	Total	C	N	O	S	0	15	0
			1190	751	210	221	8			
1	K	144	Total	C	N	O	S	0	16	0
			1198	761	209	219	9			
1	L	144	Total	C	N	O	S	0	18	0
			1209	769	212	219	9			
1	M	144	Total	C	N	O	S	0	17	0
			1201	764	210	219	8			
1	N	144	Total	C	N	O	S	0	16	0
			1198	758	211	220	9			
1	O	144	Total	C	N	O	S	0	21	0
			1221	780	212	220	9			

- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	Q	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	R	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	S	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	T	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	U	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	V	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	W	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	X	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	Y	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	Z	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	a	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	b	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	c	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	d	10	Total 221	C 100	N 50	O 61	P 10	0	10	0

- Molecule 3 is a RNA chain called RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	e	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	f	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	g	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	h	10	Total 201	C 90	N 20	O 81	P 10	0	10	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	i	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	j	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	k	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	l	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	m	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	n	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	o	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	p	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	q	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	r	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	s	10	Total 201	C 90	N 20	O 81	P 10	0	10	0

- Molecule 4 is a RNA chain called RNA (5'-R(P\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	t	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	u	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	v	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	w	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	x	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	y	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	z	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
4	1	2	Total 26	C 10	N 2	O 12	P 2	0	2	0

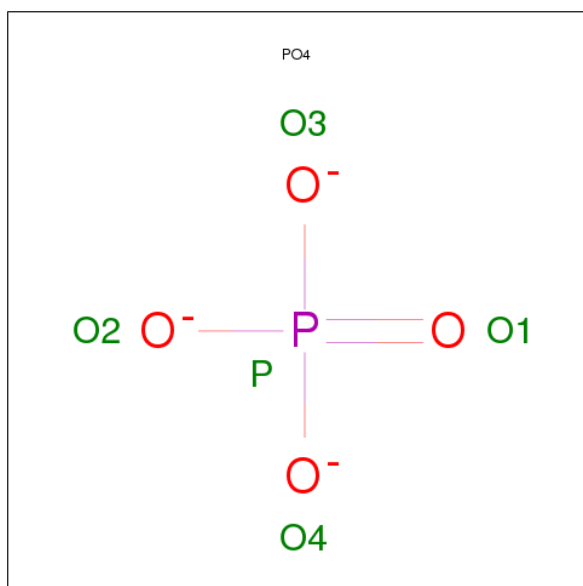
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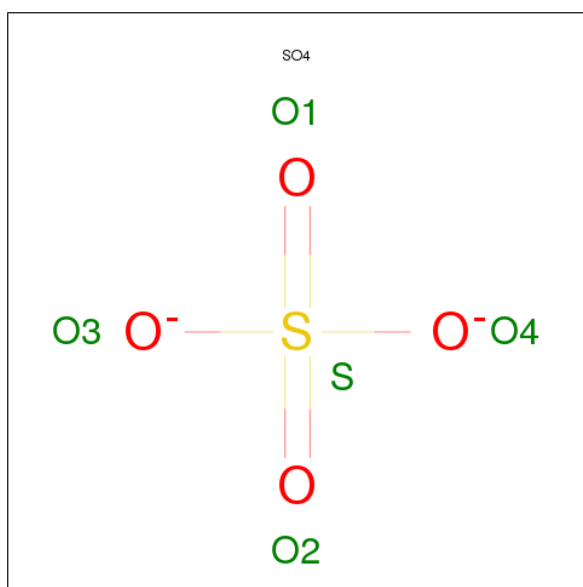
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	2	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	3	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	4	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	5	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	6	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	7	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	8	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	1
			21	20	1		
5	H	1	Total	O	P	0	1
			21	20	1		
5	N	1	Total	O	P	0	1
			21	20	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	1
			25	20	5		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	1
			25	20	5		
6	G	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	S	0	1
			25	20	5		
6	M	1	Total	O	S	0	0
			5	4	1		
6	N	1	Total	O	S	0	0
			5	4	1		
6	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Na	0	0
			1	1		
7	J	1	Total	Na	0	1
			1	1		
7	D	1	Total	Na	0	0
			1	1		
7	K	1	Total	Na	0	1
			1	1		
7	E	2	Total	Na	0	0
			2	2		
7	H	1	Total	Na	0	0
			1	1		
7	B	2	Total	Na	0	0
			2	2		
7	I	1	Total	Na	0	1
			1	1		
7	C	1	Total	Na	0	1
			1	1		
7	A	1	Total	Na	0	1
			1	1		
7	N	1	Total	Na	0	1
			1	1		
7	O	1	Total	Na	0	1
			1	1		
7	L	1	Total	Na	0	0
			1	1		
7	F	1	Total	Na	0	0
			1	1		
7	M	1	Total	Na	0	1
			1	1		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	1	Total 1	Mg 1	0	0
8	F	1	Total 1	Mg 1	0	0
8	E	1	Total 1	Mg 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	271	Total 271	O 271	0	77
9	B	267	Total 267	O 267	0	51
9	C	263	Total 263	O 263	0	43
9	D	228	Total 228	O 228	0	39
9	E	269	Total 269	O 269	0	46
9	F	259	Total 259	O 259	0	49
9	G	275	Total 275	O 275	0	49
9	H	277	Total 277	O 277	0	51
9	I	253	Total 253	O 253	0	55
9	J	279	Total 279	O 279	0	53
9	K	240	Total 240	O 240	0	60
9	L	303	Total 303	O 303	0	64
9	M	298	Total 298	O 298	0	58
9	N	254	Total 254	O 254	0	60
9	O	309	Total 309	O 309	0	70
9	P	7	Total 7	O 7	0	4

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	Q	7	Total 7	O 7	0	2
9	R	6	Total 6	O 6	0	1
9	S	8	Total 8	O 8	0	3
9	T	5	Total 5	O 5	0	1
9	U	7	Total 7	O 7	0	2
9	V	7	Total 7	O 7	0	0
9	W	6	Total 6	O 6	0	1
9	X	4	Total 4	O 4	0	2
9	Y	6	Total 6	O 6	0	1
9	Z	7	Total 7	O 7	0	2
9	a	13	Total 13	O 13	0	7
9	b	6	Total 6	O 6	0	3
9	c	6	Total 6	O 6	0	2
9	d	7	Total 7	O 7	0	2
9	e	5	Total 5	O 5	0	3
9	f	8	Total 8	O 8	0	1
9	g	9	Total 9	O 9	0	3
9	h	10	Total 10	O 10	0	2
9	i	9	Total 9	O 9	0	4
9	j	5	Total 5	O 5	0	1
9	k	9	Total 9	O 9	0	2

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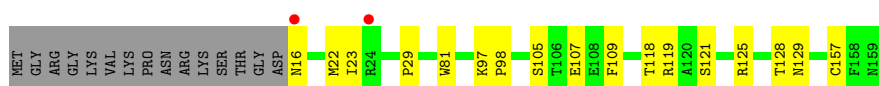
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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9	m	10	Total 10	O 10	0	4
9	n	8	Total 8	O 8	0	3
9	o	9	Total 9	O 9	0	2
9	p	6	Total 6	O 6	0	0
9	q	10	Total 10	O 10	0	4
9	r	10	Total 10	O 10	0	3
9	s	7	Total 7	O 7	0	2
9	t	1	Total 1	O 1	0	0
9	x	2	Total 2	O 2	0	0
9	4	1	Total 1	O 1	0	0
9	6	1	Total 1	O 1	0	0
9	8	1	Total 1	O 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

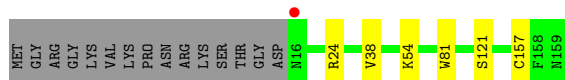
- Molecule 1: Coat protein

Chain A: 



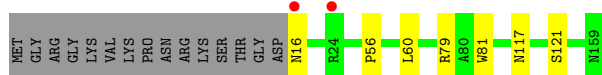
- Molecule 1: Coat protein

Chain B: 



- Molecule 1: Coat protein

Chain C: 



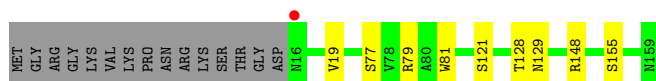
- Molecule 1: Coat protein

Chain D: 



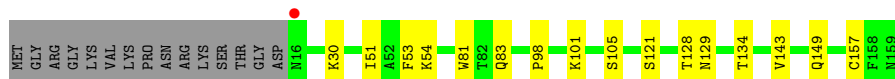
- Molecule 1: Coat protein

Chain E: 

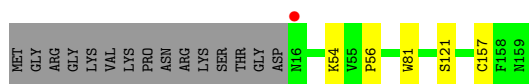


- Molecule 1: Coat protein

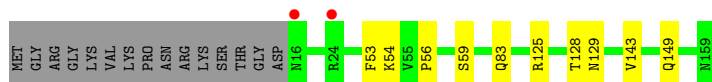
Chain F: 



- Molecule 1: Coat protein

Chain G: 

- Molecule 1: Coat protein

Chain H: 

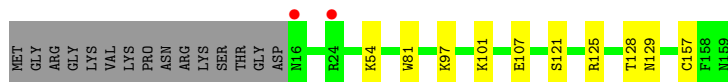
- Molecule 1: Coat protein

Chain I: 

- Molecule 1: Coat protein

Chain J: 

- Molecule 1: Coat protein

Chain K: 

- Molecule 1: Coat protein

Chain L: 

- Molecule 1: Coat protein

Chain M: 

- Molecule 1: Coat protein

Chain N: 





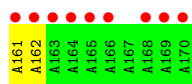
- Molecule 1: Coat protein

Chain O:



- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain P:



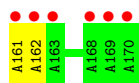
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain Q:



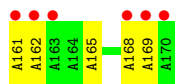
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain R:



- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain S:



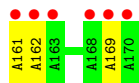
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain T:



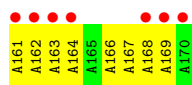
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain U:



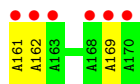
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain V: 



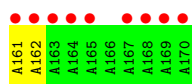
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain W: 



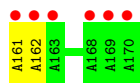
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain X: 



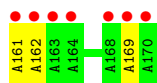
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain Y: 



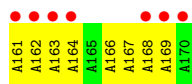
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain Z: 



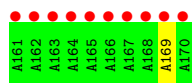
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain a: 



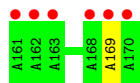
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain b: 



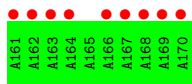
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain c: 



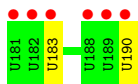
- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain d: 



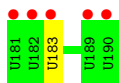
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain e: 



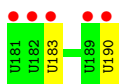
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain f: 



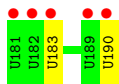
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain g: 



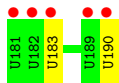
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain h: 



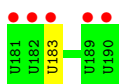
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain i: 



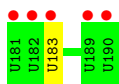
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain j: 



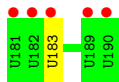
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain k: 



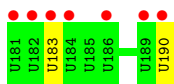
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain l:



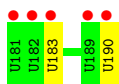
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain m:



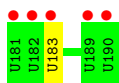
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain n:



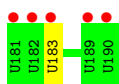
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain o:



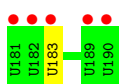
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain p:



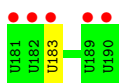
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain q:



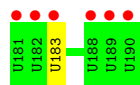
- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain r:



- Molecule 3: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')

Chain s: 



- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain t: 



- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain u: 



- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain v: 



- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain w: 



- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain x: 



- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain y: 



- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain z: 



- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain 1: 

   
  
U195  
U196

- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain 2: 

   
  
U195  
U196

- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain 3: 

   
  
U195  
U196

- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain 4: 

   
  
U195  
U196

- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain 5: 

   
  
U195  
U196

- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain 6: 

   
  
U195  
U196

- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain 7: 

   
  
U195  
U196

- Molecule 4: RNA (5'-R(P\*UP\*U)-3')

Chain 8: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.69Å 190.30Å 201.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 1.45 47.85 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.35-1.45) 98.5 (47.85-1.45)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.217 , 0.250 0.227 , 0.258	Depositor DCC
$R_{free}$ test set	28359 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 92.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	11 of 570720 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	29296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, PO4, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.58	0/1271	0.73	1/1727 (0.1%)
1	B	0.54	0/1251	0.70	0/1700
1	C	0.53	0/1284	0.71	0/1743
1	D	0.55	0/1309	0.71	0/1777
1	E	0.54	0/1286	0.70	0/1746
1	F	0.57	0/1303	0.71	0/1767
1	G	0.54	0/1266	0.68	0/1721
1	H	0.55	0/1279	0.68	0/1740
1	I	0.54	0/1272	0.72	0/1728
1	J	0.57	0/1256	0.71	0/1707
1	K	0.55	0/1273	0.72	0/1729
1	L	0.54	0/1292	0.72	0/1753
1	M	0.52	0/1274	0.71	0/1732
1	N	0.55	0/1267	0.71	0/1721
1	O	0.56	0/1306	0.70	0/1775
2	P	0.45	0/250	1.06	0/386
2	Q	0.43	0/250	1.08	0/386
2	R	0.44	0/250	1.06	0/386
2	S	0.57	0/250	1.15	1/386 (0.3%)
2	T	0.45	0/250	1.07	0/386
2	U	0.42	0/250	1.12	0/386
2	V	0.44	0/250	1.06	0/386
2	W	0.40	0/250	1.11	0/386
2	X	0.45	0/250	1.06	0/386
2	Y	0.43	0/250	1.06	0/386
2	Z	0.42	0/250	1.14	0/386
2	a	0.45	0/250	1.06	0/386
2	b	0.46	0/250	1.10	0/386
2	c	0.43	0/250	1.11	0/386
2	d	0.45	0/250	1.13	0/386
3	e	0.54	0/220	1.07	0/336
3	f	0.49	0/220	1.01	0/336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	g	0.50	0/220	1.06	0/336
3	h	0.50	0/220	1.05	0/336
3	i	0.51	0/220	1.06	0/336
3	j	0.49	0/220	1.01	0/336
3	k	0.50	0/220	1.02	0/336
3	l	0.50	0/220	1.01	0/336
3	m	0.52	0/220	1.06	0/336
3	n	0.53	0/220	1.10	0/336
3	o	0.49	0/220	1.02	0/336
3	p	0.50	0/220	1.02	0/336
3	q	0.51	0/220	1.02	0/336
3	r	0.49	0/220	1.03	0/336
3	s	0.51	0/220	1.05	0/336
4	1	0.45	0/27	0.92	0/38
4	2	0.55	0/27	1.01	0/38
4	3	0.46	0/27	0.91	0/38
4	4	0.48	0/27	1.00	0/38
4	5	0.47	0/27	0.82	0/38
4	6	0.49	0/27	1.03	0/38
4	7	0.49	0/27	1.03	0/38
4	8	0.48	0/27	0.99	0/38
4	t	0.45	0/27	0.94	0/38
4	u	0.47	0/27	1.00	0/38
4	v	0.46	0/27	0.97	0/38
4	w	0.49	0/27	0.88	0/38
4	x	0.42	0/27	0.90	0/38
4	y	0.49	0/27	0.92	0/38
4	z	0.47	0/27	0.96	0/38
All	All	0.53	0/26644	0.83	2/37466 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	165[A]	A	C3'-C2'-C1'	-6.31	96.45	101.50
1	A	119	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1201	0	1240	18	0
1	B	1191	0	1224	6	0
1	C	1204	0	1262	5	1
1	D	1223	0	1283	11	1
1	E	1211	0	1260	8	0
1	F	1216	0	1280	16	0
1	G	1198	0	1238	5	0
1	H	1205	0	1250	9	0
1	I	1201	0	1245	12	1
1	J	1190	0	1219	10	0
1	K	1198	0	1247	12	0
1	L	1209	0	1266	16	0
1	M	1201	0	1248	9	0
1	N	1198	0	1236	9	0
1	O	1221	0	1276	34	0
2	P	221	0	93	1	0
2	Q	221	0	111	1	27
2	R	221	0	111	1	0
2	S	221	0	110	2	0
2	T	221	0	96	1	0
2	U	221	0	96	2	0
2	V	221	0	111	1	27
2	W	221	0	111	1	1
2	X	221	0	111	1	0
2	Y	221	0	94	1	0
2	Z	221	0	96	2	0
2	a	221	0	111	0	26
2	b	221	0	111	0	1
2	c	221	0	111	0	1
2	d	221	0	93	0	0
3	e	201	0	83	0	0
3	f	201	0	101	0	0
3	g	201	0	101	0	0
3	h	201	0	100	0	0
3	i	201	0	83	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	j	201	0	83	0	0
3	k	201	0	101	0	0
3	l	201	0	101	0	0
3	m	201	0	101	0	0
3	n	201	0	84	0	0
3	o	201	0	83	0	0
3	p	201	0	101	0	0
3	q	201	0	101	0	0
3	r	201	0	101	0	0
3	s	201	0	82	0	0
4	1	26	0	10	5	0
4	2	26	0	10	5	0
4	3	26	0	10	1	0
4	4	26	0	10	4	0
4	5	26	0	10	5	0
4	6	26	0	10	3	0
4	7	26	0	10	2	0
4	8	26	0	10	6	0
4	t	26	0	10	0	0
4	u	26	0	10	0	0
4	v	26	0	10	0	0
4	w	26	0	10	0	0
4	x	26	0	10	0	0
4	y	26	0	10	0	0
4	z	26	0	10	0	0
5	A	21	0	0	2	0
5	H	21	0	0	0	0
5	N	21	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	E	30	0	0	0	0
6	F	5	0	0	0	0
6	G	30	0	0	0	0
6	H	5	0	0	0	0
6	I	5	0	0	0	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	0	0
6	M	30	0	0	0	0
6	N	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	5	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	K	1	0	0	0	0
9	4	1	0	0	0	0
9	6	1	0	0	0	0
9	8	1	0	0	0	0
9	A	271	0	0	7	0
9	B	267	0	0	3	0
9	C	263	0	0	1	0
9	D	228	0	0	0	0
9	E	269	0	0	1	0
9	F	259	0	0	4	0
9	G	275	0	0	1	0
9	H	277	0	0	2	0
9	I	253	0	0	4	0
9	J	279	0	0	3	0
9	K	240	0	0	3	0
9	L	303	0	0	1	0
9	M	298	0	0	2	0
9	N	254	0	0	4	0
9	O	309	0	0	5	0
9	P	7	0	0	0	0
9	Q	7	0	0	0	0
9	R	6	0	0	0	0
9	S	8	0	0	0	0
9	T	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	U	7	0	0	0	0
9	V	7	0	0	1	0
9	W	6	0	0	0	0
9	X	4	0	0	0	0
9	Y	6	0	0	0	0
9	Z	7	0	0	0	0
9	a	13	0	0	0	0
9	b	6	0	0	0	0
9	c	6	0	0	0	0
9	d	7	0	0	0	0
9	e	5	0	0	0	0
9	f	8	0	0	0	0
9	g	9	0	0	0	0
9	h	10	0	0	0	0
9	i	9	0	0	0	0
9	j	5	0	0	0	0
9	k	9	0	0	0	0
9	l	8	0	0	0	0
9	m	10	0	0	0	0
9	n	8	0	0	0	0
9	o	9	0	0	0	0
9	p	6	0	0	0	0
9	q	10	0	0	0	0
9	r	10	0	0	0	0
9	s	7	0	0	0	0
9	t	1	0	0	0	0
9	x	2	0	0	0	0
All	All	29296	0	21896	179	83

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 179 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157[B]:CYS:SG	1:J:19:VAL:HG11	1.90	1.12
1:E:19:VAL:HG11	1:K:157[B]:CYS:SG	1.99	1.02
1:D:19:VAL:HG11	1:G:157[B]:CYS:SG	2.04	0.96
1:F:51[B]:ILE:HD11	9:F:511:HOH:O	1.68	0.93
9:K:472:HOH:O	4:4:196[A]:U:C5'	2.19	0.89

The worst 5 of 83 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:a:161[A]:A:N1	2:a:169[A]:A:C2[2_555]	0.71	1.49
2:Q:161[A]:A:N1	2:Q:169[A]:A:C2[3_555]	0.72	1.48
2:V:161[A]:A:N1	2:V:169[A]:A:C2[4_555]	0.73	1.47
2:Q:162[A]:A:N6	2:Q:168[A]:A:N1[3_555]	0.88	1.32
2:V:162[A]:A:N6	2:V:168[A]:A:N1[4_555]	0.88	1.32

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/159 (99%)	153 (97%)	5 (3%)	0	100	100
1	B	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	C	160/159 (101%)	156 (98%)	4 (2%)	0	100	100
1	D	163/159 (102%)	159 (98%)	4 (2%)	0	100	100
1	E	160/159 (101%)	156 (98%)	4 (2%)	0	100	100
1	F	162/159 (102%)	157 (97%)	5 (3%)	0	100	100
1	G	158/159 (99%)	154 (98%)	4 (2%)	0	100	100
1	H	160/159 (101%)	156 (98%)	4 (2%)	0	100	100
1	I	159/159 (100%)	153 (96%)	6 (4%)	0	100	100
1	J	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	K	159/159 (100%)	155 (98%)	4 (2%)	0	100	100
1	L	161/159 (101%)	156 (97%)	5 (3%)	0	100	100
1	M	159/159 (100%)	154 (97%)	5 (3%)	0	100	100
1	N	158/159 (99%)	154 (98%)	4 (2%)	0	100	100
1	O	163/159 (102%)	158 (97%)	5 (3%)	0	100	100
All	All	2393/2385 (100%)	2325 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/140 (103%)	144 (100%)	0	100	100
1	B	142/140 (101%)	142 (100%)	0	100	100
1	C	146/140 (104%)	146 (100%)	0	100	100
1	D	149/140 (106%)	149 (100%)	0	100	100
1	E	146/140 (104%)	146 (100%)	0	100	100
1	F	148/140 (106%)	148 (100%)	0	100	100
1	G	144/140 (103%)	144 (100%)	0	100	100
1	H	146/140 (104%)	146 (100%)	0	100	100
1	I	145/140 (104%)	145 (100%)	0	100	100
1	J	143/140 (102%)	143 (100%)	0	100	100
1	K	145/140 (104%)	145 (100%)	0	100	100
1	L	147/140 (105%)	147 (100%)	0	100	100
1	M	145/140 (104%)	143 (99%)	2 (1%)	78	50
1	N	144/140 (103%)	144 (100%)	0	100	100
1	O	149/140 (106%)	149 (100%)	0	100	100
All	All	2183/2100 (104%)	2181 (100%)	2 (0%)	96	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	105[A]	SER
1	M	105[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	18	ASN
1	F	18	ASN
1	K	18	ASN
1	L	18	ASN

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Mol	Chain	Res	Type
1	M	18	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	9/10 (90%)	0	0
2	Q	9/10 (90%)	0	0
2	R	9/10 (90%)	0	0
2	S	9/10 (90%)	0	0
2	T	9/10 (90%)	0	0
2	U	9/10 (90%)	0	0
2	V	9/10 (90%)	0	0
2	W	9/10 (90%)	0	0
2	X	9/10 (90%)	0	0
2	Y	9/10 (90%)	0	0
2	Z	9/10 (90%)	0	0
2	a	9/10 (90%)	0	0
2	b	9/10 (90%)	0	0
2	c	9/10 (90%)	0	0
2	d	9/10 (90%)	0	0
3	e	9/10 (90%)	2 (22%)	0
3	f	9/10 (90%)	1 (11%)	0
3	g	9/10 (90%)	2 (22%)	0
3	h	9/10 (90%)	2 (22%)	0
3	i	9/10 (90%)	2 (22%)	0
3	j	9/10 (90%)	1 (11%)	0
3	k	9/10 (90%)	1 (11%)	0
3	l	9/10 (90%)	1 (11%)	0
3	m	9/10 (90%)	2 (22%)	0
3	n	9/10 (90%)	2 (22%)	0
3	o	9/10 (90%)	1 (11%)	0
3	p	9/10 (90%)	1 (11%)	0
3	q	9/10 (90%)	1 (11%)	0
3	r	9/10 (90%)	1 (11%)	0
3	s	9/10 (90%)	1 (11%)	0
4	1	0/2	-	-
4	2	0/2	-	-
4	3	0/2	-	-
4	4	0/2	-	-
4	5	0/2	-	-
4	6	0/2	-	-

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	7	0/2	-	-
4	8	0/2	-	-
4	t	0/2	-	-
4	u	0/2	-	-
4	v	0/2	-	-
4	w	0/2	-	-
4	x	0/2	-	-
4	y	0/2	-	-
4	z	0/2	-	-
All	All	270/330 (81%)	21 (7%)	0

5 of 21 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	e	183[A]	U
3	e	190[A]	U
3	f	183[B]	U
3	g	183[A]	U
3	g	190[A]	U

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 65 ligands modelled in this entry, 20 are monoatomic - leaving 45 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PO4	A	201[A]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	A	201[B]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	A	201[C]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	A	201[D]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	A	201[E]	8	0,0,4	0.00	-	0,0,6	0.00	-
6	SO4	A	202	-	4,4,4	0.19	0	6,6,6	0.17	0
6	SO4	B	201	-	4,4,4	0.17	0	6,6,6	0.21	0
6	SO4	C	201	-	4,4,4	0.18	0	6,6,6	0.18	0
6	SO4	D	201	-	4,4,4	0.12	0	6,6,6	0.22	0
6	SO4	E	201[A]	-	4,4,4	0.19	0	6,6,6	0.19	0
6	SO4	E	201[B]	-	4,4,4	0.22	0	6,6,6	0.20	0
6	SO4	E	201[C]	-	4,4,4	0.23	0	6,6,6	0.13	0
6	SO4	E	201[D]	-	4,4,4	0.18	0	6,6,6	0.17	0
6	SO4	E	201[E]	-	4,4,4	0.20	0	6,6,6	0.14	0
6	SO4	E	202	-	4,4,4	0.14	0	6,6,6	0.20	0
6	SO4	F	201	-	4,4,4	0.14	0	6,6,6	0.09	0
6	SO4	G	201[A]	-	4,4,4	0.24	0	6,6,6	0.21	0
6	SO4	G	201[B]	-	4,4,4	0.21	0	6,6,6	0.20	0
6	SO4	G	201[C]	-	4,4,4	0.23	0	6,6,6	0.12	0
6	SO4	G	201[D]	-	4,4,4	0.23	0	6,6,6	0.16	0
6	SO4	G	201[E]	-	4,4,4	0.24	0	6,6,6	0.16	0
6	SO4	G	202	-	4,4,4	0.21	0	6,6,6	0.11	0
5	PO4	H	201[A]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	H	201[B]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	H	201[C]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	H	201[D]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	H	201[E]	8	0,0,4	0.00	-	0,0,6	0.00	-
6	SO4	H	202	-	4,4,4	0.19	0	6,6,6	0.16	0
6	SO4	I	201	-	4,4,4	0.16	0	6,6,6	0.36	0
6	SO4	J	201	-	4,4,4	0.14	0	6,6,6	0.27	0
6	SO4	K	201	-	4,4,4	0.22	0	6,6,6	0.21	0
6	SO4	L	201	-	4,4,4	0.19	0	6,6,6	0.10	0
6	SO4	M	201[A]	-	4,4,4	0.22	0	6,6,6	0.27	0
6	SO4	M	201[B]	-	4,4,4	0.22	0	6,6,6	0.18	0
6	SO4	M	201[C]	-	4,4,4	0.22	0	6,6,6	0.12	0
6	SO4	M	201[D]	-	4,4,4	0.19	0	6,6,6	0.23	0
6	SO4	M	201[E]	-	4,4,4	0.22	0	6,6,6	0.14	0
6	SO4	M	202	-	4,4,4	0.16	0	6,6,6	0.17	0
5	PO4	N	201[A]	-	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	N	201[B]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	N	201[C]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	N	201[D]	8	0,0,4	0.00	-	0,0,6	0.00	-
5	PO4	N	201[E]	8	0,0,4	0.00	-	0,0,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	N	202	-	4,4,4	0.22	0	6,6,6	0.16	0
6	SO4	O	201	-	4,4,4	0.17	0	6,6,6	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	A	201[A]	8	-	0/0/0/0	0/0/0/0
5	PO4	A	201[B]	8	-	0/0/0/0	0/0/0/0
5	PO4	A	201[C]	8	-	0/0/0/0	0/0/0/0
5	PO4	A	201[D]	8	-	0/0/0/0	0/0/0/0
5	PO4	A	201[E]	8	-	0/0/0/0	0/0/0/0
6	SO4	A	202	-	-	0/0/0/0	0/0/0/0
6	SO4	B	201	-	-	0/0/0/0	0/0/0/0
6	SO4	C	201	-	-	0/0/0/0	0/0/0/0
6	SO4	D	201	-	-	0/0/0/0	0/0/0/0
6	SO4	E	201[A]	-	-	0/0/0/0	0/0/0/0
6	SO4	E	201[B]	-	-	0/0/0/0	0/0/0/0
6	SO4	E	201[C]	-	-	0/0/0/0	0/0/0/0
6	SO4	E	201[D]	-	-	0/0/0/0	0/0/0/0
6	SO4	E	201[E]	-	-	0/0/0/0	0/0/0/0
6	SO4	E	202	-	-	0/0/0/0	0/0/0/0
6	SO4	F	201	-	-	0/0/0/0	0/0/0/0
6	SO4	G	201[A]	-	-	0/0/0/0	0/0/0/0
6	SO4	G	201[B]	-	-	0/0/0/0	0/0/0/0
6	SO4	G	201[C]	-	-	0/0/0/0	0/0/0/0
6	SO4	G	201[D]	-	-	0/0/0/0	0/0/0/0
6	SO4	G	201[E]	-	-	0/0/0/0	0/0/0/0
6	SO4	G	202	-	-	0/0/0/0	0/0/0/0
5	PO4	H	201[A]	8	-	0/0/0/0	0/0/0/0
5	PO4	H	201[B]	8	-	0/0/0/0	0/0/0/0
5	PO4	H	201[C]	8	-	0/0/0/0	0/0/0/0
5	PO4	H	201[D]	8	-	0/0/0/0	0/0/0/0
5	PO4	H	201[E]	8	-	0/0/0/0	0/0/0/0
6	SO4	H	202	-	-	0/0/0/0	0/0/0/0
6	SO4	I	201	-	-	0/0/0/0	0/0/0/0
6	SO4	J	201	-	-	0/0/0/0	0/0/0/0
6	SO4	K	201	-	-	0/0/0/0	0/0/0/0
6	SO4	L	201	-	-	0/0/0/0	0/0/0/0
6	SO4	M	201[A]	-	-	0/0/0/0	0/0/0/0
6	SO4	M	201[B]	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	M	201[C]	-	-	0/0/0/0	0/0/0/0
6	SO4	M	201[D]	-	-	0/0/0/0	0/0/0/0
6	SO4	M	201[E]	-	-	0/0/0/0	0/0/0/0
6	SO4	M	202	-	-	0/0/0/0	0/0/0/0
5	PO4	N	201[A]	-	-	0/0/0/0	0/0/0/0
5	PO4	N	201[B]	8	-	0/0/0/0	0/0/0/0
5	PO4	N	201[C]	8	-	0/0/0/0	0/0/0/0
5	PO4	N	201[D]	8	-	0/0/0/0	0/0/0/0
5	PO4	N	201[E]	8	-	0/0/0/0	0/0/0/0
6	SO4	N	202	-	-	0/0/0/0	0/0/0/0
6	SO4	O	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	144/159 (90%)	-0.19	2 (1%) 72 78	22, 26, 33, 62	0
1	B	144/159 (90%)	-0.29	1 (0%) 84 90	22, 26, 33, 62	0
1	C	144/159 (90%)	-0.30	2 (1%) 72 78	22, 26, 32, 62	0
1	D	144/159 (90%)	-0.29	2 (1%) 72 78	22, 26, 33, 62	0
1	E	144/159 (90%)	-0.27	1 (0%) 84 90	22, 26, 33, 62	0
1	F	144/159 (90%)	-0.26	1 (0%) 84 90	22, 26, 33, 62	0
1	G	144/159 (90%)	-0.40	1 (0%) 84 90	22, 26, 33, 62	0
1	H	144/159 (90%)	-0.38	2 (1%) 72 78	22, 26, 33, 62	0
1	I	144/159 (90%)	-0.19	2 (1%) 72 78	22, 26, 33, 62	0
1	J	144/159 (90%)	-0.33	1 (0%) 84 90	22, 26, 33, 62	0
1	K	144/159 (90%)	-0.18	2 (1%) 72 78	22, 26, 33, 62	0
1	L	144/159 (90%)	-0.27	2 (1%) 72 78	22, 26, 33, 62	0
1	M	144/159 (90%)	-0.27	1 (0%) 84 90	22, 26, 33, 62	0
1	N	144/159 (90%)	-0.20	1 (0%) 84 90	22, 26, 33, 62	0
1	O	144/159 (90%)	-0.25	1 (0%) 84 90	22, 26, 33, 62	0
2	P	10/10 (100%)	10.68	9 (90%) 0 0	37, 108, 173, 178	10 (100%)
2	Q	10/10 (100%)	8.13	6 (60%) 0 0	37, 108, 173, 178	10 (100%)
2	R	10/10 (100%)	9.40	6 (60%) 0 0	37, 108, 173, 178	10 (100%)
2	S	10/10 (100%)	9.14	6 (60%) 0 0	25, 106, 185, 187	10 (100%)
2	T	10/10 (100%)	7.81	7 (70%) 0 0	36, 108, 173, 178	10 (100%)
2	U	10/10 (100%)	8.47	6 (60%) 0 0	33, 113, 176, 191	10 (100%)
2	V	10/10 (100%)	8.97	7 (70%) 0 0	37, 108, 173, 178	10 (100%)
2	W	10/10 (100%)	8.90	6 (60%) 0 0	33, 113, 176, 191	10 (100%)
2	X	10/10 (100%)	10.40	9 (90%) 0 0	37, 108, 173, 178	10 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	Y	10/10 (100%)	8.63	6 (60%) 0 0	37, 108, 173, 178	10 (100%)
2	Z	10/10 (100%)	9.54	7 (70%) 0 0	33, 113, 176, 191	10 (100%)
2	a	10/10 (100%)	10.60	7 (70%) 0 0	36, 108, 173, 178	10 (100%)
2	b	10/10 (100%)	10.79	10 (100%) 0 0	33, 113, 176, 191	10 (100%)
2	c	10/10 (100%)	9.71	6 (60%) 0 0	33, 113, 176, 191	10 (100%)
2	d	10/10 (100%)	9.83	9 (90%) 0 0	33, 113, 176, 191	10 (100%)
3	e	10/10 (100%)	4.81	6 (60%) 0 0	34, 110, 180, 198	10 (100%)
3	f	10/10 (100%)	4.11	5 (50%) 0 0	35, 109, 189, 200	10 (100%)
3	g	10/10 (100%)	4.66	5 (50%) 0 0	34, 110, 180, 198	10 (100%)
3	h	10/10 (100%)	4.15	5 (50%) 0 0	34, 110, 180, 198	10 (100%)
3	i	10/10 (100%)	4.32	5 (50%) 0 0	34, 110, 180, 198	10 (100%)
3	j	10/10 (100%)	4.62	5 (50%) 0 0	35, 109, 189, 200	10 (100%)
3	k	10/10 (100%)	4.27	5 (50%) 0 0	35, 109, 189, 200	10 (100%)
3	l	10/10 (100%)	4.59	5 (50%) 0 0	35, 109, 189, 200	10 (100%)
3	m	10/10 (100%)	5.45	7 (70%) 0 0	34, 110, 180, 198	10 (100%)
3	n	10/10 (100%)	5.11	5 (50%) 0 0	34, 110, 180, 198	10 (100%)
3	o	10/10 (100%)	4.54	5 (50%) 0 0	35, 109, 189, 200	10 (100%)
3	p	10/10 (100%)	4.77	5 (50%) 0 0	35, 109, 189, 200	10 (100%)
3	q	10/10 (100%)	5.08	5 (50%) 0 0	35, 109, 189, 200	10 (100%)
3	r	10/10 (100%)	4.59	5 (50%) 0 0	35, 109, 189, 200	10 (100%)
3	s	10/10 (100%)	5.02	6 (60%) 0 0	35, 109, 189, 200	10 (100%)
4	1	2/2 (100%)	5.25	2 (100%) 0 0	58, 58, 58, 99	2 (100%)
4	2	2/2 (100%)	5.81	2 (100%) 0 0	51, 51, 51, 100	2 (100%)
4	3	2/2 (100%)	5.58	2 (100%) 0 0	57, 57, 57, 98	2 (100%)
4	4	2/2 (100%)	4.15	2 (100%) 0 0	60, 60, 60, 95	2 (100%)
4	5	2/2 (100%)	5.96	2 (100%) 0 0	62, 62, 62, 101	2 (100%)
4	6	2/2 (100%)	5.25	2 (100%) 0 0	57, 57, 57, 96	2 (100%)
4	7	2/2 (100%)	3.61	2 (100%) 0 0	52, 52, 52, 96	2 (100%)
4	8	2/2 (100%)	5.03	2 (100%) 0 0	54, 54, 54, 98	2 (100%)
4	t	2/2 (100%)	4.24	2 (100%) 0 0	60, 60, 60, 101	2 (100%)
4	u	2/2 (100%)	5.81	2 (100%) 0 0	59, 59, 59, 99	2 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
4	v	2/2 (100%)	6.09	2 (100%)	0	0	62, 62, 62, 101	2 (100%)
4	w	2/2 (100%)	4.47	2 (100%)	0	0	70, 70, 70, 99	2 (100%)
4	x	2/2 (100%)	5.91	2 (100%)	0	0	65, 65, 65, 100	2 (100%)
4	y	2/2 (100%)	4.53	2 (100%)	0	0	70, 70, 70, 99	2 (100%)
4	z	2/2 (100%)	5.64	2 (100%)	0	0	60, 60, 60, 103	2 (100%)
All	All	2490/2715 (91%)	0.68	238 (9%)	8	9	22, 27, 130, 200	330 (13%)

The worst 5 of 238 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	a	170[A]	A	37.3
2	Z	170[B]	A	30.4
2	S	170[A]	A	27.7
2	P	161[A]	A	27.6
2	X	161[A]	A	25.9

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	M	201[E]	5/5	0.72	75.75	71,72,75,76	5
6	SO4	E	201[E]	5/5	0.55	75.52	43,44,54,55	5
6	SO4	M	201[A]	5/5	0.72	73.63	19,40,44,47	5
6	SO4	M	201[D]	5/5	0.72	72.04	33,40,48,50	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	M	201[C]	5/5	0.72	70.69	58,60,61,64	5
6	SO4	M	201[B]	5/5	0.72	70.08	72,73,76,76	5
6	SO4	E	201[A]	5/5	0.55	66.02	33,40,54,55	5
6	SO4	E	201[D]	5/5	0.55	56.24	48,49,54,54	5
6	SO4	E	201[B]	5/5	0.55	54.21	45,49,51,56	5
7	NA	N	203[A]	1/1	0.59	49.39	79,79,79,79	1
6	SO4	E	201[C]	5/5	0.55	47.10	42,45,48,51	5
6	SO4	G	201[B]	5/5	0.49	42.60	48,49,57,57	5
6	SO4	G	201[C]	5/5	0.49	41.84	31,42,53,55	5
6	SO4	G	201[A]	5/5	0.49	39.16	35,39,43,44	5
6	SO4	G	201[D]	5/5	0.49	31.54	59,60,64,65	5
7	NA	E	205	1/1	0.45	31.00	100,100,100,100	0
6	SO4	G	201[E]	5/5	0.49	30.85	54,57,58,62	5
7	NA	I	202[A]	1/1	0.32	24.22	52,52,52,52	1
7	NA	L	202	1/1	0.66	21.18	80,80,80,80	1
6	SO4	D	201	5/5	0.14	19.64	61,81,90,97	0
6	SO4	I	201	5/5	0.16	15.09	92,103,107,112	0
6	SO4	A	202	5/5	0.17	14.67	94,102,108,117	0
6	SO4	H	202	5/5	0.15	13.05	105,106,111,119	0
7	NA	C	202[B]	1/1	0.20	12.07	47,47,47,47	1
5	PO4	N	201[C]	4/5	0.15	11.77	28,29,29,31	4
5	PO4	N	201[A]	4/5	0.15	11.77	26,27,30,35	4
5	PO4	N	201[B]	4/5	0.15	11.77	17,22,32,35	4
5	PO4	N	201[D]	4/5	0.15	11.77	19,21,32,34	4
5	PO4	N	201[E]	4/5	0.15	11.77	22,30,30,35	4
6	SO4	K	201	5/5	0.18	10.40	109,116,122,125	0
6	SO4	N	202	5/5	0.22	9.52	119,121,122,130	0
6	SO4	C	201	5/5	0.14	9.12	75,86,89,98	0
6	SO4	B	201	5/5	0.20	8.99	83,99,106,111	0
7	NA	K	203[B]	1/1	0.22	8.88	43,43,43,43	1
7	NA	A	203[A]	1/1	0.14	8.49	46,46,46,46	1
6	SO4	O	201	5/5	0.14	7.96	56,78,78,89	0
7	NA	H	203	1/1	0.24	7.83	61,61,61,61	0
7	NA	D	202	1/1	0.25	7.75	103,103,103,103	0
6	SO4	F	201	5/5	0.11	7.72	58,68,75,85	0
7	NA	J	202[A]	1/1	0.17	7.30	45,45,45,45	1
7	NA	M	203[B]	1/1	0.15	7.22	41,41,41,41	1
6	SO4	L	201	5/5	0.13	7.19	87,95,100,107	0
8	MG	K	202	1/1	0.09	6.82	70,70,70,70	0
7	NA	B	203	1/1	0.17	5.29	101,101,101,101	0
5	PO4	H	201[D]	4/5	0.13	5.27	20,23,32,33	4

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PO4	H	201[A]	4/5	0.13	5.27	16,26,30,38	4
5	PO4	H	201[C]	4/5	0.13	5.27	17,25,30,33	4
5	PO4	H	201[E]	4/5	0.13	5.27	19,21,27,29	4
5	PO4	H	201[B]	4/5	0.13	5.27	19,20,30,30	4
6	SO4	M	202	5/5	0.18	5.19	77,92,97,101	0
7	NA	O	202[B]	1/1	0.12	4.23	47,47,47,47	1
6	SO4	J	201	5/5	0.16	3.73	58,80,86,89	0
5	PO4	A	201[D]	4/5	0.10	3.53	26,26,28,35	4
5	PO4	A	201[A]	4/5	0.10	3.53	22,25,26,32	4
5	PO4	A	201[C]	4/5	0.10	3.53	21,31,32,34	4
5	PO4	A	201[E]	4/5	0.10	3.53	19,28,31,32	4
5	PO4	A	201[B]	4/5	0.10	3.53	24,25,29,30	4
6	SO4	G	202	5/5	0.12	3.02	91,100,107,110	0
7	NA	E	204	1/1	0.12	2.89	64,64,64,64	0
7	NA	F	203	1/1	0.12	2.50	67,67,67,67	0
7	NA	G	203	1/1	0.11	2.47	66,66,66,66	0
8	MG	E	203	1/1	0.10	2.32	74,74,74,74	0
6	SO4	E	202	5/5	0.10	1.64	77,87,90,101	0
8	MG	F	202	1/1	0.06	-0.43	56,56,56,56	0
7	NA	B	202	1/1	0.21	-	97,97,97,97	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.